BLUE WATERS

SUSTAINED PETASCALE COMPUTING

8/14/16

# Blue Waters User Monthly Teleconference

GREAT LAKES CONSORTIUM FOR PETASCALE COMPUTATION

# Agenda

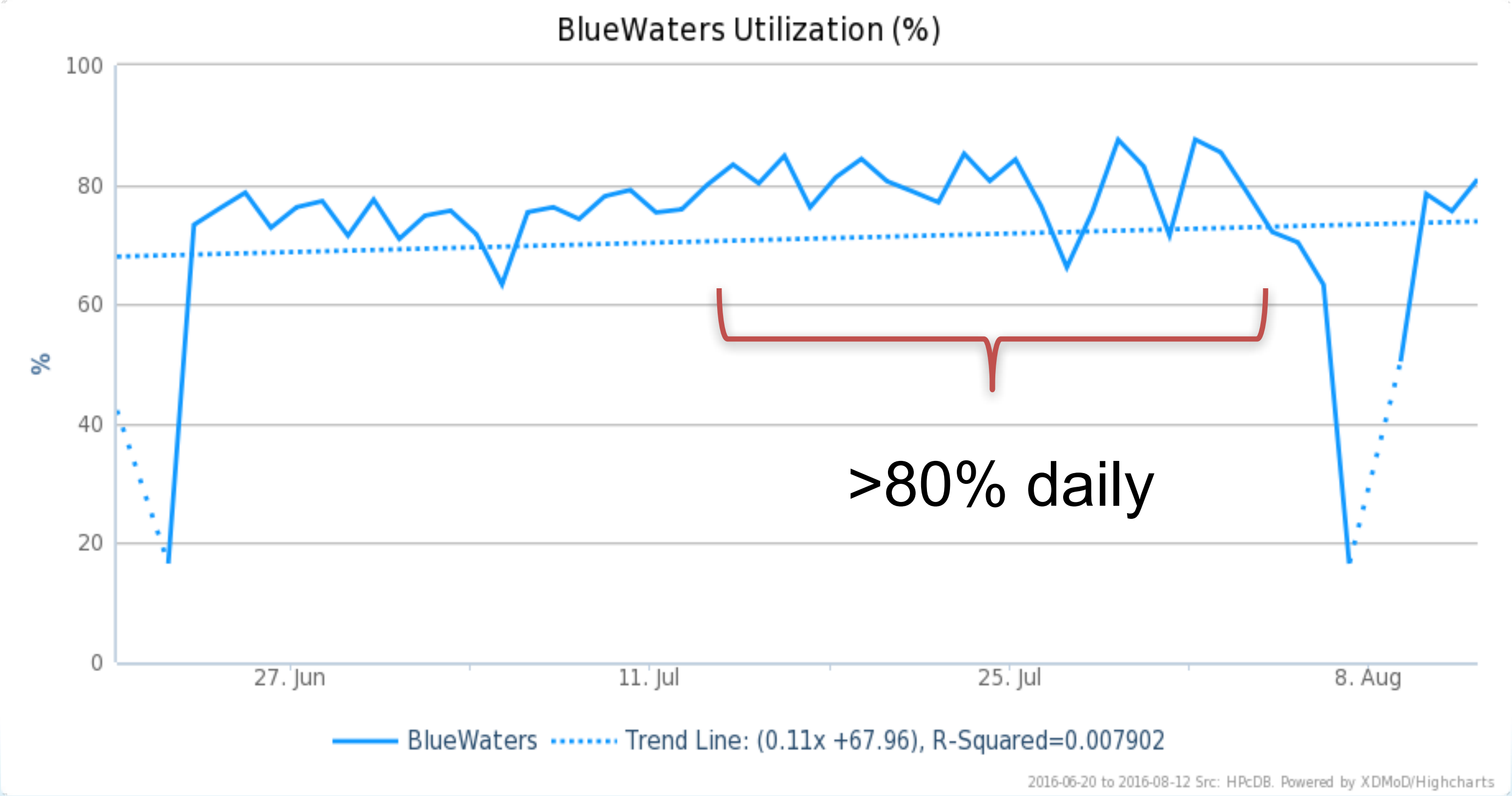
- Symposium
- File System Upgrade Status
- Maintenance Changes
- Utilization
- Recent Events
- Opportunities
- Workflow Workshop follow-up
- PUBLICATIONS!

# File System Upgrade Status

- Home & Projects file system upgrade complete. Final sync during recent maintenance.
  - soft and hard quotas to be enforced this week for home; quotas for projects to be enforced next week.
- Scratch moved to upgraded ½ file system during recent maintenance.
  - A few users had to be resynced.
  - Vendor on site this week to upgrade other ½ of scratch file system.
- Final service interruption to merge two halves of scratch.

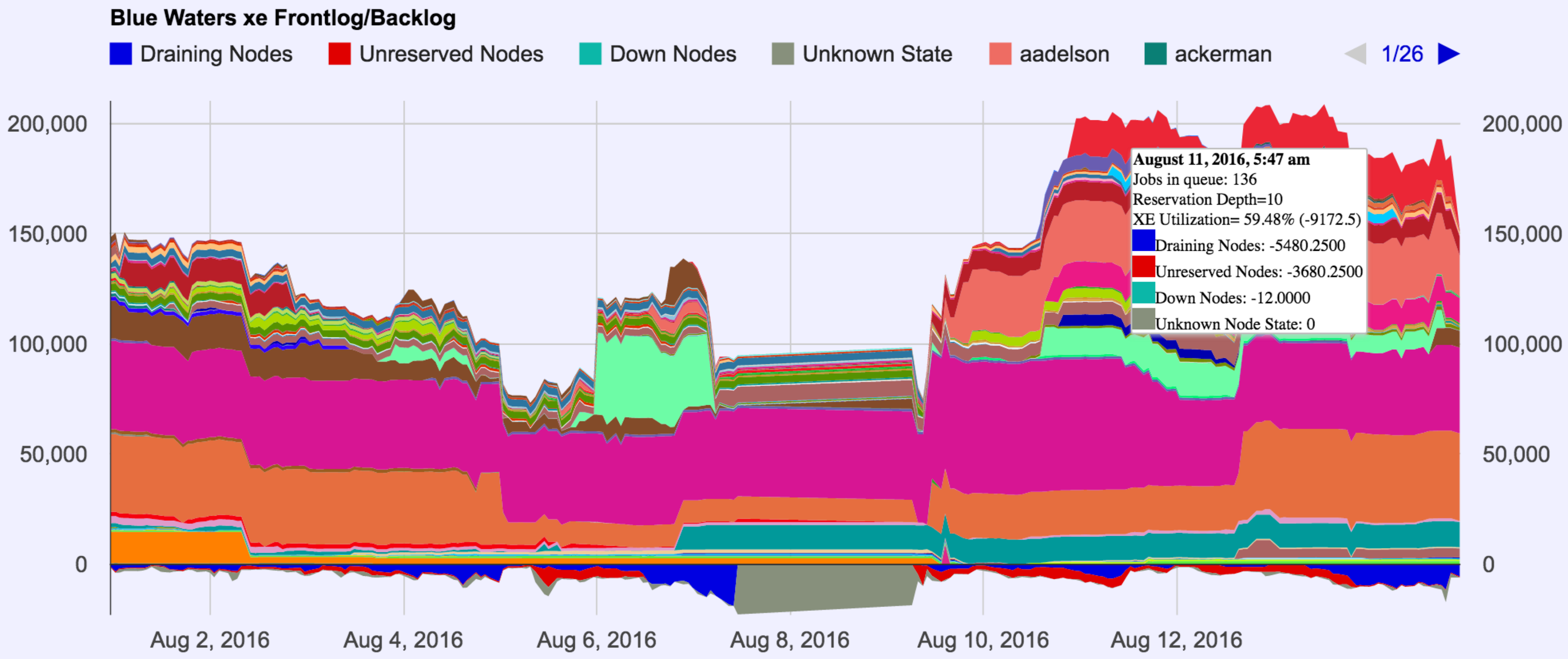
# System Utilization

- Utilization since last BW User Call (June 20)



2016-06-20 to 2016-08-12 Src: HPcDB. Powered by XDMoD/Highcharts

# Workload backlog



- Vertical axis in units of nodes.
- Plenty of jobs and varied node-hour mix

# Why isn't my job running

- Check system status page for utilization.
- Check backfill at above url or on system
  - `showbf -p bwsched -f xe`
- Check top jobs
  - `showq -i`
  - Ordered by priority. Jobs with * have a reservation on nodes.
- Check start times of jobs with reservations using `showres`.

```
> showbf -f xe -p bwsched
Partition      Tasks  Nodes      Duration   StartOffset       StartDate  Geometry
---------     ------  -----  ------------  ------------  --------------  --------
bwsched        12032    376       2:26:17      00:00:00  14:21:45_08/14  4x6x8
bwsched         7168    224       4:09:44      00:00:00  14:21:45_08/14  8x2x7
bwsched         1536     48       5:56:17      00:00:00  14:21:45_08/14  3x2x4
bwsched         1536     48       6:01:17      00:00:00  14:21:45_08/14  3x2x4
bwsched         1024     32       6:06:17      00:00:00  14:21:45_08/14  1x2x8
bwsched          640     20      INFINITY      00:00:00  14:21:45_08/14  1x2x5
```

```
> showq -i | grep -v xk | grep \*
5207970*      10321211     99.0 to  dtoussai     baea   4096     3:30:00    normal   Wed Jul 20 07:08:18
5276564*      10125901     99.0 to     yeung      jmo  16512    00:30:00      high   Wed Aug 10 20:59:04
5207973*       9587740     99.0 to  dtoussai     baea   4096     3:30:00    normal   Wed Jul 20 07:08:27
5275602*       7617711     99.0 to      guo2      jna   8000    00:30:00      high   Wed Aug 10 14:14:31
5271992*       7307965     99.0 to   pinelli      jno   9216    00:05:00      high   Tue Aug  9 13:44:27
5273294*       7200637     99.0 to   pinelli      jno  18432    00:05:00      high   Tue Aug  9 17:05:50
5246922*       5689508     99.0 to  dtoussai     baea   4096     3:30:00    normal   Sun Jul 31 01:51:04
5246923*       5642442     99.0 to  dtoussai     baea   4096     3:30:00    normal   Sun Jul 31 01:51:12
5269231*       5637764      4.9 to     clay1      jmo   8340  2:00:00:00      high   Sat Aug  6 19:06:02
5246924*       5600588     99.0 to  dtoussai     baea   4096     3:30:00    normal   Sun Jul 31 01:51:19
```

```
> showres 5207970 ...
5207970      Job I    00:33:05     4:03:05     3:30:00 4096/131072 Sun Aug 14 14:54:44
5276564      Job I     6:06:23     6:36:23    00:30:00 16512/528384 Sun Aug 14 20:28:02
5207973      Job I     2:26:23     5:56:23     3:30:00 4096/131072 Sun Aug 14 16:48:02
5275602      Job I     4:09:50     4:39:50    00:30:00 8000/256000 Sun Aug 14 18:31:29
5271992      Job I     5:56:23     6:01:23    00:05:00 9216/147456 Sun Aug 14 20:18:02
5273294      Job I     6:01:23     6:06:23    00:05:00 18432/147456 Sun Aug 14 20:23:02
5246922      Job I     6:36:23    10:06:23     3:30:00 4096/131072 Sun Aug 14 20:58:02
5246923      Job I     6:36:23    10:06:23     3:30:00 4096/131072 Sun Aug 14 20:58:02
5269231      Job I    10:06:22  2:10:06:22  2:00:00:00 8340/266880 Mon Aug 15 00:28:02
5246924      Job I  2:10:06:22  2:13:36:22     3:30:00 4096/131072 Wed Aug 17 00:28:02
```

# Recent Events

- Last week – Login node instability.
- 8/5 – Cabinet cooling failure caused cabinet EPO. Later an extended metadata server failover took place.
- 7/23 – MDS issue. Failover needed.
- 7/21 – Known lustre issue, failover cleared issue but many nodes marked down.

# Changes

- Wrapper to qsub that looks for aprun. Emits warning if not found in submitted script.
- Re-enable XALT this week. Look for MOTD and portal blog entry.
- Portal login credential expiration increased to 1 week.
- Portal “Manage Users” to require additional login check.

# Virtual School events

- Blue Waters Virtual Course Announcement
  - Introduction to High Performance Computing
  - Autumn 2016
  - Contact: Steve Gordon (sgordon@osc.edu)
  - https://www.osc.edu/~sgordon/IntroHPC
  - Instructor Dr. David E. Keyes

# Workflow Workshop

swift

Makeflow

- Over 180 registrants from 10 sites participated.
- Material available from workflow website.
- Videos to be available in 2 to 3 weeks.
- We are looking to connect teams with appropriate workloads with workflow developers.

RADICAL

Pegasus

Copernicus

Galaxy

# Review of Best Practices

- Improper use of login nodes
  - Use compute nodes for all production workloads.
- Avoid excessive calling of job scheduling commands
  - Unintentional denial of service may result otherwise.
- MOM node use should be limited to aprun launch.
  - All other commands can be run on compute nodes via aprun.
- Bundling of Jobs
  - Independent jobs bundled from 2 node to 32 nodes.
  - Avoid excessive, single nodes jobs.
  - Use a workflow.
- Small files usage
  - Use directory hierarchies, less than 10,000 files per directory.
  - Avoid many writers to same directory.
  - Tar up files before transferring to Nearline.

# Request for Science Successes

- We need to be current on products that result from time on Blue Waters such as:
  - Publications, Preprints (e.g. arXiv.org ), Presentations.
  - Very interested in data product sharing.
- Appreciate updates sooner than annual reports.
  - Send to gbauer@illinois.edu
- NSF PRAC teams send information to PoCs.
- See the Share Results section of the portal as well.
- **Be sure to include proper acknowledgment**
  - Blue Waters - National Science Foundation (ACI 1238993)
  - NSF PRAC – OCI award number